Preparation and detection of magnetic quantum phases in optical superlattices

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We describe a novel approach to prepare, detect and characterize magnetic quantum phases in ultra-cold spinor atoms loaded in optical superlattices. Our technique makes use of singlet-triplet spin manipulations in an array of isolated double well potentials in analogy to recently demonstrated quantum control in semiconductor quantum dots. We also discuss the many-body singlet-triplet spin dynamics arising from coherent coupling between nearest neighbor double wells and derive an effective description for such system. We use it to study the generation of complex magnetic states by adiabatic and non-equilibrium dynamics.

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Recent advances in the manipulations of ultra-cold atoms in optical lattices have opened new possibilities for exploring complex many-body systems [1]. A particular topic of continuous interest is the study of quantum magnetism in spin systems [2, 3, 4]. By loading spinor atoms in optical lattices it is now possible to "simulate" exotic spin models in controlled environments and to explore novel spin orders and phases.

In this Letter we describe a new approach for preparation and probing of many-body magnetic quantum states that makes use of coherent manipulation of singlet-triplet pairs of ultra-cold atoms loaded in deep period-two optical superlattices. Our approach makes use of a spin dependent energy offset between the double-well minima to completely control and measure the spin state of two-atom pairs, in a way analogous to the recently demonstrated manipulations of coupled electrons in semiconductor double-dots [5]. As an example, we show how this technique allows one to detect and analyze anti-ferromagnetic spin states in optical lattices. We further study the many-body dynamics that emerge when tunneling between nearest neighbor double wells is allowed. As two specific examples, we show how a set of singlet atomic states can be evolved into singlet-triplet cluster-type states and into a maximally entangled superposition of two anti-ferromagnetic states. Finally, we discuss the use of our projection technique to probe the density of spin defects (kinks) in magnetic states prepared via equilibrium and non-equilibrium dynamics.

The key idea of this work is illustrated by considering a pair of ultra-cold atoms with two relevant internal states, which we identify with spin up and down $\sigma =\uparrow,\downarrow$ in an isolated double well (DW) potential as shown in Fig.1. By dynamically changing the optical lattice parameters, it is possible to completely control this system and measure it in an arbitrary two-spin basis. For concreteness, we first focus on the fermionic case. The physics of this system is governed by three sets of energy scales: i) the on-site interaction energy $U = U_{\uparrow\downarrow}$ between the atoms, ii) the tunneling energy of the σ species: J_σ, and iii) the energy difference between the two DW minima, $2\Delta_\sigma$ for each of the two species. The σ index in J and Δ is due to the fact that the lattice that the $\uparrow$ and $\downarrow$ atoms feel can be engineered to be different by choosing laser beams of appropriate polarizations, frequencies, phases and intensities. In the following we assume that the atoms are strongly interacting, $U \gg J_\sigma$, and that effective vibrational energy of each well, $\hbar\omega_0$, is the largest energy scale in the system $\hbar\omega_0 \gg U, \Delta_\sigma, J_\sigma$, i.e deep wells.

Singlet $|s\rangle$ and triplet $|t\rangle$ states form the natural basis for the two-atom system. The relative energies of these states can be manipulated by controlling the energy bias Δ_σ between the two wells. In the unbiased case ($U \gg 2\Delta_\sigma$) only states with one atom per site $(1, 1)$ are populated, as the large atomic repulsion energetically suppresses double occupancy (here, labels (m, n) indicate the integer number of atoms in the left and right sites of the DW). For weak tunneling and spin independent lattices ($J_\uparrow = J_\downarrow = J$, $\Delta_\uparrow = \Delta_\downarrow = \Delta$) the states $(1, 1)|s\rangle$ and $(1, 1)|t\rangle$ are nearly degenerated. The small energy splitting between them is $\sim 4J^2/U$, with the singlet being the low energy state (Fig. 1a). As Δ is increased the relative energy of doubly occupied states $(0, 2)$ decreases. Therefore, states $(1, 1)|s\rangle$ and $(0, 2)|s\rangle$ will hybridize. When $2\Delta \gtrsim U$ the atomic repulsion is overwhelmed and consequently the $(0, 2)|s\rangle$ becomes the ground state. At the same time, Pauli exclusion results in a large energy splitting $\hbar\omega_0$ between doubly occupied singlet and triplet states as the latter must have an antisymmetric orbital wave function. Hence, $(1, 1)|t\rangle$ does not hybridize with its doubly occupied counterpart, and its relative energy becomes large as compared to the singlet state. Thus the energy difference between singlet and triplet states can be controlled using Δ.

Further control is provided by changing J_σ and Δ_σ in spin dependent lattices (see Fig.1b). Specifically, let us now consider the regime $2\Delta_\sigma \ll U$ in which only $(1, 1)$ subspace is populated. Within this manifold we define [6]

$$|s\rangle = \hat{s}^\dagger|0\rangle \equiv \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle), \quad (1)$$

$$|t_z\rangle = \hat{t}_z^\dagger|0\rangle \equiv \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \quad (2)$$

$$|t_x\rangle = \hat{t}_x^\dagger|0\rangle \equiv \frac{-1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle), \qquad (3)$$

$$|t_y\rangle = \hat{t}_y^\dagger|0\rangle \equiv \frac{i}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) \qquad (4)$$

Here $\hat{t}_\alpha^\dagger$ and $\hat{s}$ are operators that create triplet and singlet states from the vacuum $|0\rangle$ (state with no atoms). They satisfy bosonic commutation relations and the constrain $(\sum_{\alpha=x,y,z}\hat{t}_\alpha^\dagger\hat{t}_\alpha) + \hat{s}^\dagger\hat{s} = 1$, due to the physical restriction that the state in a double well is either a singlet or a triplet. In the rest of the letter we will omit the label $(1,1)$ for the singly occupied states.

When Δ_σ depends on spin, i.e $\Upsilon \equiv \Delta_\uparrow - \Delta_\downarrow \neq 0$, the $|t_z\rangle$ component mixes with $|s\rangle$(see Fig.1c). Note that on the other hand $|t_{x,y}\rangle$ remain decoupled from $|t_z\rangle$ and $|s\rangle$. As a result the states $|s\rangle$ and $|t_z\rangle$ form an effective two-level system whose dynamics is driven by the Hamiltonian:

$$\hat{H}_1^J = -\zeta(\hat{s}^\dagger\hat{s} - \hat{t}_z^\dagger\hat{t}_z) - \Upsilon\tilde{S}^z + \text{const}, \qquad (5)$$

Here $\zeta \equiv 2J_\uparrow J_\downarrow/\tilde{U}$, is the exchange coupling energy (with $\tilde{U} \equiv \frac{U^2-(\Delta_\uparrow+\Delta_\downarrow)^2}{U}$) and $\tilde{S}^z = \hat{s}^\dagger\hat{t}_z + \hat{t}_z^\dagger\hat{s}$. If $\Upsilon = 0$, exchange dominates and $|s\rangle$ and $|t_z\rangle$ becomes the ground and first excited states respectively. However if $\Upsilon \gg \zeta$, exchange can be neglected and the ground state becomes either $|\uparrow\downarrow\rangle$ or $|\downarrow\uparrow\rangle$ depending on the sign of Υ.

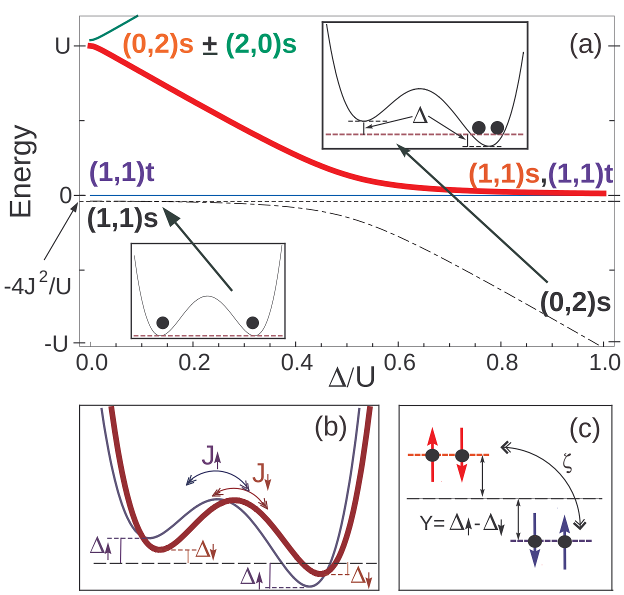

FIG. 1: (color online) a) Energy levels of fermionic atoms in a spin independent double well as Δ/U is varied: While in the regime $2\Delta \ll U$, $(1,1)|s\rangle$ is the lowest energy state, when $2\Delta \gtrsim U$, $(0,2)|s\rangle$ becomes the state with lowest energy. b) In spin dependent potentials the two species feel different lattice parameters c) Restricted to the $(1,1)$ subspace Υ acts as an effective magnetic field gradient and couples the $|s\rangle$ and $|t_z\rangle$ states .

These considerations indicate that it is possible to perform arbitrary coherent manipulations and robust measurement of atom pair spin states. The former can be accomplished by combining time-dependant control over ζ, Υ to obtain effective rotations on the spin-$1/2$ Bloch sphere within $|s\rangle - |t_z\rangle$ state. In the parameter regime of interest, ζ, Υ, can be varied independently in experiments. In addition, by applying pulsed (uniform) magnetic fields it is possible to rotate the basis, thereby changing the relative population of the $|t_{x,y,z}\rangle$ states. Atom pair spin states can be probed by adiabatically increasing Δ until it becomes larger than $U/2$, in which case atoms in the $|s\rangle$ will adiabatically follow to $(0,2)|s\rangle$ while the atoms in $|t_\alpha\rangle$ will remain in (1,1) state (Fig. 1a). A subsequent measurement of the number of doubly occupied wells will reveal the number of singlets in the initial state. Such a measurement can be achieved by efficiently converting the doubly occupied wells into molecules via photoassociation or using other techniques such as microwave spectroscopy and spin changing collisions [7]. Alternatively, one can continue adiabatically tilting the DW until it merges to one well. In such a way the $|s\rangle$ will be projected to the $(0,2)|s\rangle$, while the triplets will map to $(0,2)|t_\alpha\rangle$. As $(0,2)|t_\alpha\rangle$ has one of the atoms in the first vibrational state of the well, by measuring the population in excited bands one can detect the number of initial $|t_\alpha\rangle$ states. Hence the *spin-triplet blockade* [5] allows to effectively control and measure atom pairs.

Detection and diagnostics of many-body spin phases such as antiferromagnetic (AF) states is an example of direct application of the singlet-triplet manipulation and measurement technique. The procedure to measure the AF state population is the following; after inhibiting tunneling between the various DWs, one can abruptly increase Υ, such that the initial state is projected into the new eigenstates $|\uparrow\downarrow\rangle$ and $|\downarrow\uparrow\rangle$ at time $\tau = \tau_0$. For $\tau > \tau_0$ Υ can then be adiabatically decreased to zero, in which case the $|\uparrow\downarrow\rangle$ pairs will be adiabatically converted into $|s\rangle$ and $|\downarrow\uparrow\rangle$ pairs to $|t_z\rangle$. Finally, the singlet population can be measured using the spin blockade. As a result, a measure of the doubly occupied sites (or excited bands population) will detect the number of $|\uparrow\downarrow\rangle$ pairs and thus probe antiferromagnetic states of the type $|\uparrow\downarrow\uparrow\downarrow\ldots\rangle$.

These ideas can be directly generalized to perform measurements of the more complex magnetic states that can be represented as products of two atom pairs. For example, a pulse of RF magnetic field can be used to orient all spins, thus providing the ability to detect $|AF\rangle$ states aligned along an arbitrary direction. Moreover, one can determine the relative phase between singlet and triplet pairs in $|AF\rangle$ states of the form $\prod|s\rangle + e^{i\phi}|t_z\rangle$ by performing Ramsey-type spectroscopy. After letting the system evolve freely (with $\Upsilon = 0$) so that the $|s\rangle$ and $|t_z\rangle$ components accumulate an additional relative phase due to exchange, a read-out pulse (controlled by pulsing Υ) will map the accumulated phase onto population of singlet and triplet pairs. To know ϕ is important as it determines the direction of the anti-ferromagnetic order. Furthermore, by combining the blockade with noise correlation measurements [8] it is possible to obtain further information about the magnetic phases. While the blockade probes local correlation in the DWs, noise measurements probe non-local

spin-spin correlations and thus can reveal long range order.

Before proceeding we note that similar ideas to that outlined above can be used for bosonic atoms if initially no $|t_{x,y}\rangle$ states are populated. The latter can be done by detuning the $|t_{x,y}\rangle$ states by means of an external magnetic field. In the bosonic case the doubly occupied t_z states will be the ones that have the lowest energy. They will be separated by an energy $\hbar\omega_0$ from the doubly occupied singlets as the latter are the ones that have antisymmetric orbital wave function in bosons. Consequently, the role of $|s\rangle$ in fermions will be replaced by $|t_z\rangle$ in bosons. The read-out procedure would then be identical to that described above, while the coherent dynamics will be given by the Hamiltonian Eq.(5) apart from the sign change $\zeta \to -\zeta$.

Up to now our analysis has ignored tunneling between different DWs, but in practice this tunneling can be controlled by tuning the lattice potential. How will singlet and triplet pairs evolve due to this coupling? We will now discuss the many-body dynamics that emerges when nearest neighbor DW tunneling is allowed, i.e. $t_\sigma > 0$. When atoms can hop between DWs, the behavior of the system will depend on the dimensionality. For simplicity we will restrict our analysis to a 1D array of N double-wells, where t_σ corresponds to hopping energy of σ-type atoms between the right site of the $j^{th} - DW$ and the left site of the $(j+1)^{th} - DW$.

In the regime $J_\sigma, t_\sigma, \Delta_\sigma \ll U$, multiply occupied wells are energetically suppressed and the effective Hamiltonian is given by $\hat{H}^{eff} = \hat{H}_J + \hat{H}_t$. Here the first term corresponds to the sum over N independent H_j^J Hamiltonians (see Eq.(5)), $\hat{H}_J = \sum_{j=1}^N H_j^J$, each of which acts on its respective j^{th}-DW. On the other hand $\hat{H}_t$ is non-local as it couples different DWs and quartic as it consists of terms with four singlet-triplet operators [9]. The coupled DWs system is in general complex and the quantum spin dynamics can be studied only numerically. However, there are specific parameter regimes where an exact solution can be found. For this discussion we will set $\Delta_\sigma = 0$. If $t_\uparrow/t_\downarrow \to 0$, and at time $\tau = 0$, no $|t_x\rangle, |t_y\rangle$ triplet states are populated, their population will remain always zero. Consequently, in this limit, the relevant Hilbert space reduces to that of an effective spin one-half system with $|s\rangle$ and $|t_z\rangle$ representing the effective $\pm 1/2$ states, which we denote as $|\Uparrow\rangle$ and $|\Downarrow\rangle$. $\hat{H}_t$ couples such effective spin states. In the restricted Hilbert space $\hat{H}^{eff}$ maps exactly to an Ising chain in a magnetic field:

$$\hat{H}^{eff} = \mp\zeta \sum_j \hat{\sigma}_j^z - \lambda_z \sum_j \hat{\sigma}_j^x \hat{\sigma}_{j+1}^x \tag{6}$$

where $\hat{\sigma}^\alpha$ are the usual Pauli matrices which act of the effective $|\Uparrow\rangle$ and $|\Downarrow\rangle$ spins. In terms of singlet-triplet operators they are given by $\hat{\sigma}_j^z = (\hat{s}_j^\dagger \hat{s}_j - \hat{t}_{zj}^\dagger \hat{t}_{zj})$, $\hat{\sigma}_j^x = \hat{s}_j^\dagger \hat{t}_{zj} + \hat{t}_{zj}^\dagger \hat{s}_j$ and $\hat{\sigma}_j^y = (\hat{s}_j^\dagger \hat{t}_{zj} - \hat{t}_{zj}^\dagger \hat{s}_j)/i$. Here $\lambda_z = \frac{t_\downarrow^2}{2U} - \frac{t_\downarrow^2}{U_{\downarrow\downarrow}}$ and the upper and lower signs are for fermions and bosons respectively. For fermions in the lowest vibrational level the onsite interaction energy between the same type of atoms $U_{\uparrow\uparrow}, U_{\downarrow\downarrow} \to \infty$ due to the Pauli exclusion principle.

The 1D quantum Ising model exhibits a second order quantum phase transition at the critical value $|g| \equiv |\lambda_z/\zeta| = 1$. For fermions (upper sign) when $g \ll 1$ the ground state corresponds to all effective spins pointing up, i.e $|G\rangle = |\Uparrow \dots \Uparrow\rangle = \Pi_j |s\rangle_j$. On the other hand when $g \gg 1$, there are two degenerate ground states which are, in the effective spin basis, macroscopic superpositions of oppositely polarized states along x. In terms of the original fermionic spin states this superposition correspond to the states $|AF^\pm\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow \dots \uparrow\downarrow\rangle \pm |\downarrow\uparrow \dots \downarrow\uparrow\rangle)$. Therefore, by adiabatic passage one could start with $|G\rangle$ and convert it into AF state(s). Due to vanishing energy gap at the quantum critical point $g = 1$, adiabaticity is difficult to maintain as $N \to \infty$ [11, 12, 13, 14]. In that respect, our projection scheme is useful to test adiabatic following. It can be done either by measuring the number of $|\uparrow\downarrow\rangle$ pairs in the final state or by adiabatically ramping down g back to zero and measuring the number of singlets/triplet pairs. The remaining number of triplets will determine the number of excitations created in the process.

We now turn to non-adiabatic dynamics. We will discuss the situation where initially the system is prepared in a product of singlet states ($\lambda_z = 0$ ground state) and then one lets it evolve for $\tau > 0$ with a fixed $|\lambda_z| > 0$. Generically the coupling between DWs results in oscillations between singlet and triplet pairs with additional decay on a slower time scale. We present two important special cases involving such dynamics:

i) *Singlet-triplet cluster state generation:* If the value of λ_z is set to be $|\lambda_z| \gg \zeta$, then the Hamiltonian reduces to a pure Ising Hamiltonian and thus at particular times, τ_c, given by $\lambda_z \tau_c/\hbar = \pi/4 \bmod \pi/2$ the evolving state becomes a $d = 1$ cluster state $|\mathcal{C}\rangle$ in the effective spin basis [15]. Up to single spin rotations $|\mathcal{C}\rangle = \frac{1}{2^{N/2}} \bigotimes_{j=1}^N (|\Uparrow\rangle_j \hat{\sigma}_{j+1}^z + |\Downarrow\rangle_j)$. Cluster states are of interest for the realization of one-way quantum computation proposals where starting from the state $|\mathcal{C}\rangle$ computation can be done via measurements only. Preparation of cluster states encoded in the logical $\Uparrow, \Downarrow$ qubits may have significant practical advantages since the $\Uparrow, \Downarrow$ states have zero net spin along the quantization axis and hence are not affected by global magnetic field fluctuations. Additionally, the use of such singlet-triplet states for encoding might allow for the generation of decoherence free subspaces insensitive to collective and local errors [16] and for alternative schemes for measured-based quantum computation [17].

ii) *Non-equilibrium generation and probing of AF correlations:* The second situation is when the value of λ_z is set to the critical value, $|\lambda_z| = \zeta$ (or $g = 1$). We will first focus on the fermionic system $\lambda_z > 0$. To discuss it, we remind that the dynamics driven by $\hat{H}^{eff}$ is exactly solvable as $\hat{H}^{eff}$ can be mapped via the Jordan Wigner transformation into a quadratic Hamiltonian of fermionic operators which can be diagonalized by a canonical transformation [10, 14]. Using such transformation it is possible to show that at specific times, the shortest of them we denote by $\tau_m \approx \hbar\frac{N+1}{4\zeta}$, long range AF correlations build up and for small atom number the state approaches $|AF^+\rangle$. To quan-

tify the resulting state in Fig. 2(inset) we plot the fidelity, defined as $\mathcal{F}_1(\tau_m) = |\langle AF^+|\psi(\tau_m)\rangle_{g=1}|^2$, as a function of N. The figure shows that while an almost perfect $|AF^+\rangle$ is dynamically generated for small N, its fidelity exponentially degrades with increasing atom number.

However, the fidelity is a very strict probe, as it drops to zero when a single spin is flipped. As N increases the system ends at τ_m in a quantum superposition of states like $|\cdots \Rightarrow\Leftarrow\Leftarrow\Leftarrow\Leftarrow\Leftarrow\Rightarrow\Rightarrow\Rightarrow\Rightarrow\Rightarrow\Rightarrow\Leftarrow \quad \dots \rangle$ with finite domains of "effective spins" pointing along $\pm x$, separated by kinks where the polarization of the spins change its orientation (we used the convention $|\uparrow\downarrow\rangle \equiv |\Rightarrow\rangle$). Consequently, one gets more realistic information about the AF order of the state, by measuring the average size of the domains or the average density of kinks, the latter defined as $\nu \equiv \frac{1}{2N}\sum_j(1 - \langle\psi(\tau)|\hat{\sigma}_j^x\hat{\sigma}_{j+1}^x|\psi(\tau)\rangle)$.

Our read-out technique can be used to detect the kink-density as for an arbitrary fixed g energy conservation imposes a relation between ν and the triplet-z density, N_t:

$$\nu(\tau, g) = \frac{1}{2} - \frac{N_t(\tau, g)}{g}. \qquad (7)$$

A simple analytical expression for $N_t(\tau, g)$ can be obtained by using the Jordan Wigner transformation [10]: $N_t(\tau, g) = \frac{1}{N}\lambda_z^2\sum_{k=0}^{N-1}\frac{\sin^2(2\pi k/N)\sin^2(2\omega_k\tau)}{\hbar^2\omega_k^2}$ where $\hbar\omega_k = \zeta\sqrt{g^2 + 1 + 2g\cos(2\pi k/N)}$ are quasi-particle frequencies of $\hat{H}^{eff}$. The fact that it remains always below 0.2 (see Fig. 2) confirms the idea that regardless of the reduced fidelity at large N, the state does retain AF correlations. We point out that $|AF^+\rangle$ states are only generated at $g = 1$, a feature that illustrates the special character of the critical dynamics.

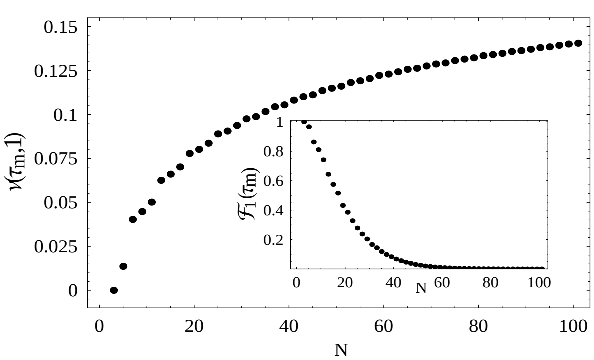

FIG. 2: Using the the Jordan-Wigner transformation [10] we calculated the density of kinks *vs* N at $\tau = \tau_m$ and the fidelity $|\langle\psi(\tau_m)|AF^+\rangle|^2$ *vs* N (inset). Our projection technique can be used to measure $\nu(\tau)$ as it is directly related to the triplet density, $N_t(\tau)$ (see Eq.(7)).

Let us now discuss the bosonic case. If $\lambda_z > 0$, the fermionic results apply for bosons by simply interchanging the role of $|s\rangle \leftrightarrow |t_z\rangle$. On the other hand if $\lambda_z < 0$, not only one has to interchange $|s\rangle \leftrightarrow |t_z\rangle$ but additionally, the adiabatic and non-equilibrium dynamics will generate, instead of $|AF^{\pm}\rangle$ states, $\frac{1}{\sqrt{2}}(|\Rightarrow\Leftarrow \cdots \Rightarrow\Leftarrow\rangle \pm |\Leftarrow\Rightarrow \cdots \Leftarrow\Rightarrow\rangle)$ i.e macroscopic superpositions of AF states along the x-direction in the effective spin basis. With these modifications, the results derived for fermions hold for bosons[21].

Before concluding we briefly mention that spin dependent superlattices of the form

$$V = \sum_{j=1,2}(A_j + B_j\sigma_z)\cos^2[kz/j + \theta_j] \qquad (8)$$

can be experimentally realized by superimposing two independent lattices, generated by elliptically polarized light, one with twice the periodicity of the other [18, 19, 20]. Complete control over the DW parameters is achieved by controlling the phases (which determine Δ), intensities (which determine U,J and t) and polarization of the laser beams (which allow for spin dependent control). For example lattice configurations with $t_\uparrow \ll t_\downarrow$ can be achieved by setting the laser parameters such that $B_1 = 0$ and $A_2 = B_2 \gg 1$.

In summary we have described a technique to prepare, detect and manipulate spin configurations in ultra-cold atomic systems loaded in spin dependent period-two superlattices. By studying the many-body dynamics that arises when tunneling between DWs is allowed, we discussed how to dynamically generate singlet-triplet cluster states and AF cat states, which are of interest for quantum information science, and how to probe AF correlations in far from equilibrium dynamics. Even though in this Letter we restrict our analysis to 1D systems the ideas developed here can be extended to higher dimensions and more general kinds of interactions.

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[21] In this case a different sign in the definition of kink density $\hat{\sigma}_j^x \hat{\sigma}_{j+1}^x \to -\hat{\sigma}_j^x \hat{\sigma}_{j+1}^x$ is required.